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Drahoslava Janovská and Gerhard Opfer

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Linear equations in quaternions

Drahoslava Janovská[1] and Gerhard Opfer[2]

[1] Institute of Chemical Technology, Prague, Technická 5, 166 28 Prague 6, Czech Republic janovskd@vscht.cz
[2] University of Hamburg, MIN Faculty, Department of Mathematics, Bundesstraße 55, 20146 Hamburg, Germany opfer@math.uni-hamburg.de

Summary. The aim is to solve a linear equation in quaternions namely, the equation $\sum_{j=1}^{j=\nu} a^{(j)} x b^{(j)} = e$, where $a^{(j)}$, $b^{(j)}$ and e are given quaternions, the quaternion x stands for the unknown solution. We give an algorithm based on a fixed point formulation.

1 Basic properties and definitions for quaternions

We start with some information on the algebra of quaternions. There are more details in our previous papers [4], [8]. General information is contained in books, like [3], [7]. Results concerning matrices with quaternion elements are surveyed in [10]. Applications to quantum mechanics are treated in [1], [2], and applications in chemistry are given in [9].

We denote by $\mathbb{H} = \mathbb{R}^4$ the skew field of quaternions. Let $a = (a_1, a_2, a_3, a_4)$, $b = (b_1, b_2, b_3, b_4) \in \mathbb{H}$. Then, addition is defined elementwise and multiplication is governed by the following rule:

$$\begin{aligned} ab := (&a_1b_1 - a_2b_2 - a_3b_3 - a_4b_4, a_1b_2 + a_2b_1 + a_3b_4 - a_4b_3, \\ &a_1b_3 - a_2b_4 + a_3b_1 + a_4b_2, a_1b_4 + a_2b_3 - a_3b_2 + a_4b_1). \end{aligned} \tag{1}$$

The first component a_1 of $a = (a_1, a_2, a_3, a_4) \in \mathbb{H}$ is called the *real part* of a and denoted by $\Re a$. The second component a_2 is called the *imaginary part* of a and denoted by $\Im a$. A quaternion $a = (a_1, 0, 0, 0)$ will be identified with $a_1 \in \mathbb{R}$ and $a = (a_1, a_2, 0, 0)$ will be identified with $a_1 + \mathrm{i}a_2 \in \mathbb{C}$. The zero element $(0, 0, 0, 0) \in \mathbb{H}$ and the unit element $(1, 0, 0, 0) \in \mathbb{H}$ will be abbreviated by $0, 1$, respectively. Let $a = (a_1, a_2, a_3, a_4) \in \mathbb{H}$. The *conjugate* of a, denoted by $\overline{a}$, will be defined by

$$\overline{a} := (a_1, -a_2, -a_3, -a_4).$$

The *absolute value* of a, denoted by $|a|$, will be defined by

$$|a| := \sqrt{a_1^2 + a_2^2 + a_3^2 + a_4^2}.$$

There are the following important rules:

$$\begin{aligned}
\Re(ab) &= \Re(ba), \\
|ab| &= |ba| = |a||b|, \\
|a|^2 &= a\,\overline{a} = \overline{a}\,a, \\
\overline{a\,b} &= \overline{b}\,\overline{a}, \\
a^{-1} &= \frac{\overline{a}}{|a|^2},\ a \neq 0, \\
(a\,b)^{-1} &= b^{-1}\,a^{-1},\ a, b \neq 0.
\end{aligned}$$

We denote by $\mathbb{H}^n$ the normed vector space of n-vectors formed by quaternions, where the norm of $\mathbf{x} := (x_1, x_2, \ldots, x_n) \in \mathbb{H}^n$ will be defined by

$$||\mathbf{x}|| := \sqrt{|x_1|^2 + |x_2|^2 + \cdots + |x_n|^2}.$$

Let $\mathbb{H}^{m\times n}$ be the set of all $(m \times n)$-matrices with elements from $\mathbb{H}$. We note here, that these matrices act as *linear mappings* $\ell : \mathbb{H}^n \to \mathbb{H}^m$ only in the following sense:

$$\begin{aligned}
\ell(\mathbf{x} + \mathbf{y}) &= \ell(\mathbf{x}) + \ell(\mathbf{y}), \quad \mathbf{x}, \mathbf{y} \in \mathbb{H}^n, \\
\ell(\mathbf{x}\alpha) &= \ell(\mathbf{x})\alpha, \quad \mathbf{x} \in \mathbb{H}^n,\ \alpha \in \mathbb{H}.
\end{aligned}$$

The converse is also true: A linear mapping ℓ defined by the above two properties is always represented by a matrix. This follows from standard arguments.

Let $\mathbf{A} \in \mathbb{H}^{m\times n}$. By $\mathbf{A}^{\mathrm{T}} \in \mathbb{H}^{n\times m}$ we understand the *transposed matrix* of $\mathbf{A}$ where the rows and columns are exchanged. By $\overline{\mathbf{A}} \in \mathbb{H}^{m\times n}$ we understand the matrix which is formed by conjugation of all its elements. Finally,

$$\mathbf{A}^* := (\overline{\mathbf{A}})^{\mathrm{T}} = \overline{\mathbf{A}^{\mathrm{T}}}.$$

In case $\mathbf{A}^* = \mathbf{A}$, we call $\mathbf{A}$ *Hermitean*. The zero element of $\mathbb{H}^n$ and of $\mathbb{H}^{m\times n}$ will be denoted by $\mathbf{0}$. From the context it will become clear which zero element is meant. A matrix $\mathbf{A} \in \mathbb{H}^{n\times n}$ will be called *unitary* if $\mathbf{A}^*\mathbf{A} = \mathbf{A}\mathbf{A}^* = \mathbf{I}$, where $\mathbf{I}$ is the identity matrix. Unitary matrices $\mathbf{A}$ are characterized by $||\mathbf{A}\mathbf{x}|| = ||\mathbf{x}||$ for all $\mathbf{x} \in \mathbb{H}^n$.

Eigenvalue problems for $\mathbf{A} \in \mathbb{H}^{n\times n}$ have to be posed in the form

$$\mathbf{A}\mathbf{x} = \mathbf{x}\lambda \tag{2}$$

and similar matrices have the same set of eigenvalues. The set of eigenvalues is in general not finite. If λ is an eigenvalue, the whole *equivalence class*

$$[\lambda] := \left\{\sigma \in \mathbb{H} : \sigma = h\lambda h^{-1} \text{ for all } h \in \mathbb{H}\backslash\{0\}\right\}$$

consists of eigenvalues. The number of different equivalence classes is, however, at most n.

Lemma 1. *Two quaternions λ_1 and λ_2 are members of the same equivalence class if and only if $|\lambda_1| = |\lambda_2|$ and $\Re\lambda_1 = \Re\lambda_2$. As a consequence, two different complex numbers are equivalent if and only if they are conjugate two each other. Two real numbers are equivalent if and only if they coincide.*

Proof: See [4]. □

This lemma implies that in any equivalence class $[q]$ of quaternions there is exactly one complex quaternion $\tilde{q}$ with $\Re\tilde{q} \geq 0$. This will be called the *complex representative* of $[q]$. If $q = (q_1, q_2, q_3, q_4) \in [q]$, then $\tilde{q} = (q_1, \sqrt{q_2^2 + q_3^2 + q_4^2}, 0, 0)$ is the complex representative of $[q]$.

We should note here, that Hermitean matrices have only real eigenvalues and that all eigenvalues λ of unitary matrices obey $|\lambda| = 1$.

2 Linear equations in quaternions

With the intention to obtain some insight for a forthcoming study of the multidimensional case, we study here first the simplest case with a linear equation in one variable.

At first, let us recall the following general matrix theorem.

Theorem 1. *Let $\mathbf{A}$ be a real, square matrix with the property*

$$\mathbf{A} + \mathbf{A}^{\mathrm{T}} = 2c\mathbf{I},$$

where $\mathbf{I}$ is the identity matrix of the same size as $\mathbf{A}$ and $c \in \mathbb{R}$. Then,

$$\Re\lambda(\mathbf{A}) = c$$

for all eigenvalues λ of $\mathbf{A}$.

Corollary 1. *Under the assumptions of the previous theorem let $c \neq 0$. Then, $\mathbf{A}$ is nonsingular.*

In the following equation, the two vectors $\mathbf{a} := (a^{(1)}, a^{(2)}, \ldots, a^{(\nu)})$, $\mathbf{b} := (b^{(1)}, b^{(2)}, \ldots, b^{(\nu)}) \in \mathbb{H}^\nu$, $\nu \in \mathbb{N}$, and the *right hand side* $e \in \mathbb{H}$ are given and $x \in \mathbb{H}$ stands for the unknown solution:

$$L^{(v)}(x) := \sum_{j=1}^{\nu} a^{(j)} x b^{(j)} = e, \quad e, x \in \mathbb{H},\ a^{(j)}, b^{(j)} \in \mathbb{H}\backslash\{0\},\ j = 1, \ldots, \nu. \tag{3}$$

The mapping $L^{(\nu)} : \mathbb{H} \to \mathbb{H}$ is additive, i. e. $L^{(\nu)}(x+y) = L^{(\nu)}(x) + L^{(\nu)}(y)$, but not homogeneous in general, i. e. $L^{(\nu)}(\alpha x) \neq \alpha L^{(\nu)}(x)$ and $L^{(\nu)}(x\alpha) \neq L^{(\nu)}(x)\alpha$, $x \in \mathbb{H}$, $\alpha \in \mathbb{H}$. To call equation (3) a *linear equation* (for a fixed $\nu > 1$) is thus true only in a restricted sense. Without loss of generality, we assume that $a^{(1)} = b^{(\nu)} = 1$. So we have for $\nu = 1, 2, 3$ (simplifying the notation slightly)

$$L^{(1)}(x) := x; \quad L^{(2)}(x) := ax + xb; \quad L^{(3)}(x) := ax + cxd + xb. \tag{4}$$

Since the unknown x resides in the middle between c and d, we will call all terms of the type cxd *middle terms*. The problem $L^{(2)}(x) = e$ was treated, probably for the first time by Johnson in [6]. It is easy to find an explicit solution formula for $L^{(2)}(x) := ax + xb = e$. We assume that neither a nor b is real (including zero). We multiply $ax + xb = e$ from the left by $\overline{a}$ and from the right by $\overline{b}$ and divide by $|a|^2$ ($|b|^2$ would be possible, too). Then we add this equation to the original equation and obtain after some simple algebraic operations

$$\left(2\Re b + a + \frac{|b|^2}{|a|^2}\,\overline{a}\right) x = e + \frac{\overline{a} e \overline{b}}{|a|^2}.$$

Lemma 2. *Let* $a = (a_1, a_2, a_3, a_4)$, $b = (b_1, b_2, b_3, b_4)$. *Equation* $L^{(2)}(x) = e$ *(cf.* (4)*) has a unique solution for all choices of* e *if and only if* $a_1 + b_1 \neq 0$ *or* $\sum_{j=2}^{4}(a_j^2 - b_j^2) \neq 0$.

Proof: For simplicity in the sequel we put

$$s = a + b, \quad d = a - b. \tag{5}$$

Let the j-th component of s, d be denoted by s_j, d_j, respectively, $j = 1, 2, 3, 4$. If we use the multiplication rule (1), then $ax + xb = e$ is equivalent to the real 4×4 system

$$\mathbf{A}\mathbf{x} = \mathbf{e}, \quad \mathbf{A} := \begin{pmatrix} s_1 & -s_2 & -s_3 & -s_4 \\ s_2 & s_1 & -d_4 & d_3 \\ s_3 & d_4 & s_1 & -d_2 \\ s_4 & -d_3 & d_2 & s_1 \end{pmatrix}, \tag{6}$$

where $\mathbf{x}, \mathbf{e} \in \mathbb{R}^4$ have to be identified with $x, e \in \mathbb{H}$, respectively. We compute the determinant of $\mathbf{A}$ and find

$$\det(\mathbf{A}) = s_1^2(s_1^2 + s_2^2 + s_3^2 + s_4^2 + d_2^2 + d_3^2 + d_4^2) + (s_2 d_2 + s_3 d_3 + s_4 d_4)^2. \quad (7)$$

The determinant vanishes if and only if $s_1 := a_1 + b_1 = 0$ and $s_2 d_2 + s_3 d_3 + s_4 d_4 := a_2^2 + a_3^2 + a_4^2 - (b_2^2 + b_3^2 + b_4^2) = 0$. □

For solving the system (6), we compute the determinants of the j-th minors $\mathbf{A}_j := \mathbf{A}_{(1:j,1:j)}$, $j = 1, 2, 3$: $\det(\mathbf{A}_1) = s_1$, $\det(\mathbf{A}_2) = s_1^2 + s_2^2$, $\det(\mathbf{A}_3) = s_1\left(s_1^2 + s_2^2 + s_3^2 + d_4^2\right)$. We see that $s_1 \neq 0$ implies that all four determinants (including that of $\mathbf{A}$) do not vanish, which implies that Gauss' elimination process can be carried out without pivoting. If however, $s_1 = 0$, the first and third minor have a vanishing determinant. In this case pivoting is necessary.

Corollary 2. *In the previous lemma let* (i) $a = b$*. The equation* $L^{(2)}(x) = e$ *(see* (4)*) has a unique solution if and only if* $a_1 = \Re a \neq 0$*. If* $a_1 = 0$ *but* $a \neq 0$ *the kernel of* $\mathbf{A}$ *is a two dimensional subspace of* $\mathbb{R}^4$. (ii) *Let* $|a| = |b| \neq 0$*. In this case* $\mathbf{A}$*, defined in* (6) *is singular if and only if* $s_1 = a_1 + b_1 = 0$*. If* $s_1 = 0$ *the kernel of* $\mathbf{A}$ *is a two dimensional subspace of* $\mathbb{R}^4$*, provided* $a, b \notin \mathbb{R}$.

Proof: We use formula (7). (i) In this case $d := a - b = 0$ implies $\det(\mathbf{A}) = 16 a_1^2 |a|^2$, where $\mathbf{A}$ is defined in (6). If $a_1 = 0$, then

$$\mathbf{A} = 2\begin{pmatrix} 0 & -a_2 & -a_3 & -a_4 \\ a_2 & 0 & 0 & 0 \\ a_3 & 0 & 0 & 0 \\ a_4 & 0 & 0 & 0 \end{pmatrix}. \quad (8)$$

(ii) In this case we have $\det(\mathbf{A}) = 4|a|^2(a_1 + b_1)^2$ and $s_1 = 0$ implies

$$\mathbf{A} = \begin{pmatrix} 0 & -s_2 & -s_3 & -s_4 \\ s_2 & 0 & -d_4 & d_3 \\ s_3 & d_4 & 0 & -d_2 \\ s_4 & -d_3 & d_2 & 0 \end{pmatrix}. \quad (9)$$

Since $\mathbf{A} + \mathbf{A}^{\mathrm{T}} = \mathbf{0}$, Theorem 1 implies that all four eigenvalues of $\mathbf{A}$ have vanishing real part. Since the eigenvalues appear pairwise conjugate, the rank of $\mathbf{A}$ is either 0, 2 or 4. If $\operatorname{rank}(\mathbf{A}) = 0$, then, $a_j = b_j = 0, j = 2, 3, 4$ and $a, b \in \mathbb{R}$. The case $\operatorname{rank}(\mathbf{A}) = 4$ was already excluded. A formula for the two dimensional kernel was given in [4]. □

The matrix $\mathbf{A}$ of (6) has the property that $\mathbf{A} + \mathbf{A}^{\mathrm{T}} = 2(a_1 + b_1)\mathbf{I}$, where $\mathbf{I}$ is the (4×4) identity matrix. Theorem 1 implies that all eigenvalues of $\mathbf{A}$

have the same real part $a_1 + b_1$ and it implies (Corollary 1) that $a_1 + b_1 \neq 0$ is a sufficient condition for $\mathbf{A}$ being non singular.

We will develop a simple iterative algorithm for solving $L^{(2)}(x) := ax + xb = e$ in the original form under the assumption that both $a \neq 0, b \neq 0$. If $a = 0$ or $b = 0$, then finding the solution is trivial. We form two fixed point equations by multiplying $L^{(2)}(x) := ax + xb = e$ from the left by a^{-1} and another one by multiplying from the right by b^{-1}. This yields

$$T_1(x) := a^{-1}(e - xb) = x, \quad T_2(x) := (e - ax)b^{-1} = x. \tag{10}$$

Lemma 3. *Let $L^{(2)}(x) := ax + xb = e$ have a unique solution $\hat{x}$, regardless of the choice of e. Let $a \neq 0, b \neq 0$. If* (i) *$|a| > |b|$, let $q := |b|/|a| < 1$. The fixed point equation $T_1(x) = x$ is contractive and the sequence $\{x_j\}$ defined by $x_{j+1} := T_1(x_j)$, $j = 0, 1, \ldots$ converges with geometric speed to the solution $\hat{x}$ regardless of the choice of the initial guess x_0. There is the error estimate*

$$|\hat{x} - x_j| \leq \min\left\{\frac{q^j}{1-q}|x_1 - x_0|, \frac{q}{1-q}|x_j - x_{j-1}|\right\}, \ j \geq 1.$$

If (ii) *$|a| < |b|$, let $q := |a|/|b|$. Then, the same is true for T_2.*

Proof: We treat the case (i). Then, $|T_1(x) - T_1(y)| = |a^{-1}(y - x)b| = |a^{-1}|\,|b|\,|x - y| = q|x - y|$. The remaining part follows from standard arguments. Case (ii) is analogue. □

Example 1. Take $a := (-2, -4, 7, -10)$, $b := (5, 9, 10, 6)$, $e := (-1, 0, -6, 3)$. Then, $q := |a|/|b| = 0.8357$, $\hat{x} = (-0.02825\,79443\,1218, 0.52768\,86450\,6780, -0.04595\,79753\,6487, 0.23548\,28692\,6819)$. Iteration with T_2 yields $|\hat{x} - x_{100}| \approx 9.3 \cdot 10^{-9}$ with error estimate $|\hat{x} - x_{100}| \leq 4.2 \cdot 10^{-8}$.

If $|a| = |b|$ and $a_1 + b_1 \neq 0$ the above iterations will in general not converge. If $|a|, |b|$ are different but close together, the convergence will be very slow.

We turn now to the case $L^{(3)}(x) = e$ where $L^{(3)}$ is defined in (4). Put $c = (c_1, c_2, c_3, c_4)$, $d = (d_1, d_2, d_3, d_4)$, $x = (x_1, x_2, x_3, x_4)$ and identify the column vector $\mathbf{x}$ with x. Then, the middle term cxd can be expressed as

$$cxd = \mathbf{M}\mathbf{x}, \qquad \text{where}$$

$$\mathbf{M} := \left(\begin{array}{ll} c_1d_1 - c_2d_2 - c_3d_3 - c_4d_4 & -c_1d_2 - c_2d_1 + c_3d_4 - c_4d_3 \\ c_1d_2 + c_2d_1 + c_3d_4 - c_4d_3 & c_1d_1 - c_2d_2 + c_3d_3 + c_4d_4 \\ c_1d_3 - c_2d_4 + c_3d_1 + c_4d_2 & -c_1d_4 - c_2d_3 - c_3d_2 + c_4d_1 \\ c_1d_4 + c_2d_3 - c_3d_2 + c_4d_1 & c_1d_3 - c_2d_4 - c_3d_1 - c_4d_2 \end{array}\right.$$

$$\left.\begin{matrix} -c_1d_3 - c_2d_4 - c_3d_1 + c_4d_2 & -c_1d_4 + c_2d_3 - c_3d_2 - c_4d_1 \\ c_1d_4 - c_2d_3 - c_3d_2 - c_4d_1 & -c_1d_3 - c_2d_4 + c_3d_1 - c_4d_2 \\ c_1d_1 + c_2d_2 - c_3d_3 + c_4d_4 & c_1d_2 - c_2d_1 - c_3d_4 - c_4d_3 \\ -c_1d_2 + c_2d_1 - c_3d_4 - c_4d_3 & c_1d_1 + c_2d_2 + c_3d_3 - c_4d_4 \end{matrix}\right) \in \mathbb{R}^{4\times 4}.$$

Let us remark that $\det \mathbf{M} = |c|^2|d|^2 \neq 0$ if both $c \neq 0$ and $d \neq 0$. If $c = 0$ or $d = 0$, we come back to $L^{(2)}(x) = e$.

With $\mathbf{A}$ from (5), (6), the final (4×4) system has the form

$$(\mathbf{A} + \mathbf{M})\mathbf{x} = \mathbf{e}.$$

Under the assumption that all a, b, c and d are nonzero quaternions, the matrix $\mathbf{A} + \mathbf{M}$ is regular (we proved it by making use of Maple).

Similarly as in the previous case, we form this time three fixed point equations: we multiply $L^{(3)}(x) := ax + cxd + xb = e$ from the left by a^{-1} or multiply $L^3(x)$ from the right by b^{-1}. The last equation we obtain by multiplying the equation $cxd = e - ax - xb$ from the left by c^{-1} and from the right by d^{-1}. This yields

$$T_1(x) := a^{-1}(e - cxd - xb) = x, \quad T_2(x) := (e - cxd - ax)b^{-1} = x, \tag{11}$$

$$T_3(x) := c^{-1}(e - ax - xb)d^{-1} = x. \tag{12}$$

Lemma 4. *Let $L^{(3)}(x) := ax + cxd + xb = e$ have a unique solution $\hat{x}$, regardless of the choice of e. Let $a \neq 0$, $b \neq 0$, $c \neq 0$, $d \neq 0$. If* (i) *$|a| > |b|$ and $|c||d| < |a| - |b|$, let $q := \dfrac{|c||d| + |b|}{|a|} < 1$. The fixed point equation $T_1(x) = x$ is contractive and the sequence $\{x_j\}$ defined by $x_{j+1} := T_1(x_j)$, $j = 0, 1, \ldots$ converges with geometric speed to the solution $\hat{x}$ regardless of the choice of the initial guess x_0.* If (ii) *$|a| < |b|$ and $|c||d| < |b| - |a|$, let $q := \dfrac{|c||d| + |b|}{|a|} < 1$. Then, the same is true for T_2. If* (iii) *$|a| + |b| < |c||d|$, let $q := \dfrac{|a| + |b|}{|c||d|} < 1$. Then the fixed point equation $T_3(x) = x$ is contractive and the sequence $\{x_j\}$ defined by $x_{j+1} := T_3(x_j)$, $j = 0, 1, \ldots$ converges to the solution $\hat{x}$ regardless of the choice of the initial guess x_0.*

In all three cases, the error estimate is

$$|\hat{x} - x_j| \leq \min\left\{\frac{q^j}{1-q}|x_1 - x_0|, \frac{q}{1-q}|x_j - x_{j-1}|\right\}, j \geq 1.$$

Proof: We treat the case (iii). Then,

$$|T_3(x) - T_3(y)| = |c^{-1}(a(y-x) + (y-x)b)d^{-1}| = |c|^{-1}|a(y-x) + (y-x)b| \leq$$
$$\leq |c|^{-1}|d|^{-1}(|a(y-x)| + |(y-x)b|) = |c|^{-1}|d|^{-1}(|a||y-x| + |b||y-x|) =$$
$$= |c|^{-1}|d|^{-1}(|a| + |b|)|y-x| = q|x-y|.$$

The remaining part follows from standard arguments. Case (i) and (ii) is analogue to the proof of Lemma 3. □

Let us remark that the equation $ax + cxd + xb = e$ can be also transformed into the system of two equations for two unknown quaternions by introducing a new variable $u = cxd$:

$$\begin{aligned} ax + u + xb &= e \\ c^{-1}u - xd &= 0. \end{aligned} \tag{13}$$

For the general case of $L^{(\nu)}(x) = e$ introduced in (3) all middle terms define a matrix $\mathbf{M}_j$ of exactly the form of $\mathbf{M}$ so that the general case expressed as real equivalent is of the form

$$(\mathbf{A} + \sum_{j=2}^{\nu-1} \mathbf{M}_j)\mathbf{x} = \mathbf{e}. \tag{14}$$

The general case can also be transformed into a system of $\nu - 1$ equations in $\nu - 1$ unknowns by putting $u_j := a^{(j)}xb^{(j)}, j = 2, 3, \ldots, \nu - 1$. The system has then, the following form (assuming $a^{(1)} = b^{(\nu)} = 1$):

$$\begin{aligned} xb^{(1)} + u_2 + u_3 + \cdots + u_{\nu-1} + a^{(\nu)}x &= e, \\ (a^{(2)})^{-1}u_2 - xb^{(2)} &= 0, \\ (a^{(3)})^{-1}u_3 - xb^{(3)} &= 0, \\ &\vdots \\ (a^{(\nu-1)})^{-1}u_{\nu-1} - xb^{(\nu-1)} &= 0. \end{aligned} \tag{15}$$

We have multiplications from the left and from the right, but there are no middle terms with multiplication from the left and from the right, simultaneously.

Let us remark that the situation is more complicated in the general case of linear systems in quaternions. For example we have to define multiplication of the matrix by a quaternion from the left, to introduce left and right eigenvalues, etc. The aim of our future work will be to develop an algorithm (similar to the elimination procedure) for solving these systems.

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